

10/561,969A Yong Chu 10-12-2007

\$%^STN;HighlightOn=;HighlightOff=;

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PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 13:04:28 ON 12 OCT 2007
FILE 'CAPLUS' ENTERED AT 13:04:28 ON 12 OCT 2007
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COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	338.12	1071.62
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-46.80	-49.14

=> file reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	338.12	1071.62
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-46.80	-49.14

FILE 'REGISTRY' ENTERED AT 13:04:42 ON 12 OCT 2007
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STRUCTURE FILE UPDATES: 11 OCT 2007 HIGHEST RN 950420-07-2
DICTIONARY FILE UPDATES: 11 OCT 2007 HIGHEST RN 950420-07-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

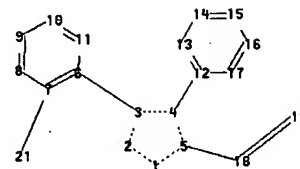
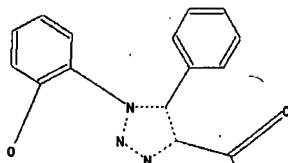
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REGISTRY includes numerically searchable data for experimental and
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chain nodes :

18 19 20 21

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17

chain bonds :

3-6 4-12 5-18 7-21 18-19 18-20

ring bonds :

1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11 12-13 12-17 13-14 14-15

15-16 16-17

exact/norm bonds :

1-2 1-5 2-3 3-4 3-6 4-5 7-21 18-19 18-20

exact bonds :

4-12 5-18

normalized bonds :

6-7 6-11 7-8 8-9 9-10 10-11 12-13 12-17 13-14 14-15 15-16 16-17

G1:O,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS

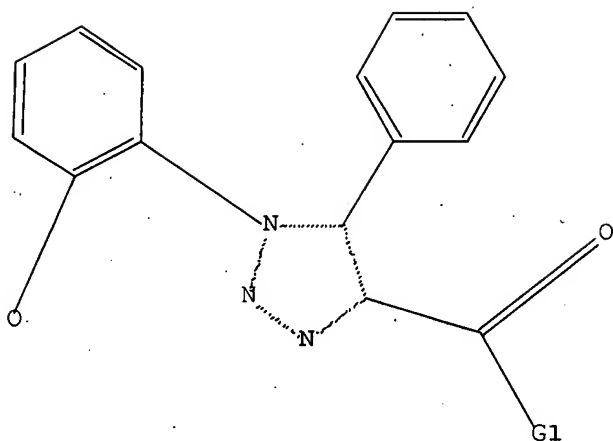
20:CLASS 21:CLASS

L24 STRUCTURE UPLOADED

=> d

L24 HAS NO ANSWERS

L24 STR



G1 O,N

Structure attributes must be viewed using STN Express query preparation.

=> s 124

SAMPLE SEARCH INITIATED 13:05:07 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 6 TO ITERATE

100.0% PROCESSED 6 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 6 TO 266
PROJECTED ANSWERS: 0 TO 0

L25 0 SEA SSS SAM L24

=> s 124 full

FULL SEARCH INITIATED 13:05:18 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 152 TO ITERATE

100.0% PROCESSED 152 ITERATIONS 13 ANSWERS
SEARCH TIME: 00.00.01

L26 13 SEA SSS FUL L24

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.55	1244.17
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-49.14

FILE 'CAPLUS' ENTERED AT 13:06:00 ON 12 OCT 2007

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FILE COVERS 1907 - 12 Oct 2007 VOL 147 ISS 17
FILE LAST UPDATED: 11 Oct 2007 (20071011/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

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=> s l26

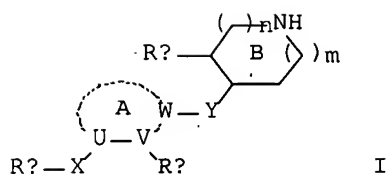
L27 4 L26

=> d ibib abs hitstr tot

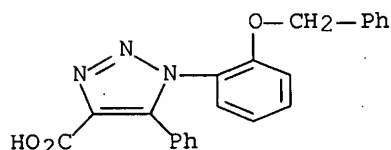
L27 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:935063 CAPLUS Full-text
DOCUMENT NUMBER: 147:301199
TITLE: Preparation of cyclic amine compounds as renin inhibitors
INVENTOR(S): Kuroita, Takanobu; Imaeda, Yasuhiro; Taya, Naohiro; Oda, Tsuneo; Iwanaga, Kouichi; Asano, Yasutomi
PATENT ASSIGNEE(S): Takeda Pharmaceutical Company Limited, Japan
SOURCE: PCT Int. Appl., 587pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007094513	A2	20070823	WO 2007-JP53242	20070215
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			

PRIORITY APPLN. INFO.: US 2006-774133P P 20060216
OTHER SOURCE(S): MARPAT 147:301199
GI



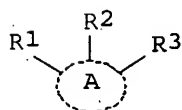
- AB The title compds. N-(pyrrol-3-ylcarbonyl)piperazine and N-(imidazol-4-ylcarbonyl)piperazine, and N-(pyrazol-3-ylcarbonyl)piperazine, and N-(2-pyridylcarbonyl)piperazines represented by the formula [I; ring A = 5- or 6-membered arom. heterocycle optionally having substituent (s); U, V, W = each independently C or N, provided that when any one of U, V and W is N, then the others should be C; Ra, Rb = independently cyclic group, C1-10 alkyl, C2-10 alkenyl, or C2-10alkynyl each optionally having substituent (s); X = a bond, or a spacer having 1 to 6 atoms in the main chain; Y = a spacer having 1 to 6 atoms in the main chain; Rc = hydrocarbon group optionally contg. heteroatom(s) as the constituting atom(s), which optionally has substituent(s); m, n = independently 1 or 2; ring B optionally further has substituent(s)] or salts thereof are prepd. These compds. have excellent renin inhibitory activity, and thus is useful as agents for the prophylaxis or treatment of hypertension or various organ damages attributable to hypertension. Thus, a soln. of 1-(3-morpholinophenyl)-5-phenyl-1H-imidazole-4-carboxylic acid 262, (3R)-1,3-dibenzylpiperazine 200, WSC.HCl 173, and HOBt 122 mg, 5 mL DMF was stirred at room temp. for 15 h, followed by hydrogenolysis over 20% Pd(OH)₂ on carbon in methanol and treatment with HCl in Et₂O/EtOAc to give 4-[3-[4-[(2R)-2-benzylpiperazin-1-yl]carbonyl]-5-phenyl-1H-imidazol-1-yl]phenylmorpholine dihydrochloride (II). II inhibited human renin (prepn. given) by 103 and 104% at 1 and 10 μ M, resp. A tablet formulation contg. (2R)-1-[(1,2-Diphenyl-1H-pyrrol-3-yl)carbonyl]-2-(2-phenylethyl)piperazine hydrochloride was prepd.
- IT 947271-58-1P, 1-[2-(Benzyloxy)phenyl]-5-phenyl-1H-1,2,3-triazole-4-carboxylic acid
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate; prepn. of cyclic amine compds. as renin inhibitors for prophylaxis or treatment of hypertension)
- RN 947271-58-1 CAPLUS
- CN 1H-1,2,3-Triazole-4-carboxylic acid, 5-phenyl-1-[2-(phenylmethoxy)phenyl]-
 (CA INDEX NAME)



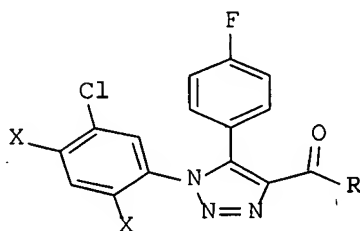
DOCUMENT NUMBER: 142:114071
 TITLE: Preparation of substituted 5-membered ring compounds as heat shock protein 90 (HSP90) inhibitors
 INVENTOR(S): Cheung, Kwai Ming; Dymock, Brian William; MacDonald, Edward; Drysdale, Martin James
 PATENT ASSIGNEE(S): Vernalis Cambridge Limited, UK; Cancer Research Technology Ltd.; The Institute of Cancer Research
 SOURCE: PCT Int. Appl., 49 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005000300	A1	20050106	WO 2004-GB2755	20040624
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1638555	A1	20060329	EP 2004-743106	20040624
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
US 2006235058	A1	20061019	US 2006-561969	20060410
PRIORITY APPLN. INFO.:			GB 2003-15111	A 20030627
			WO 2004-GB2755	W 20040624
OTHER SOURCE(S):			MARPAT 142:114071	
GI				

Current app.



I



II

AB Title compds. I [wherein A = 5-membered cycle; R1 = (un)substituted (hetero)aryl; R2 (adjacent to R1) = absence, H, carboxamide, (un)substituted (hetero)aryl, carbocycle or heterocycle; R3 (adjacent to R2) = absence, H, (un)substituted cycloalky(en)yl, alk(en/yn)yl, carboxyl, carboxamide or ester; with some limitations, or salts, N-oxides, hydrates or solvates thereof] were

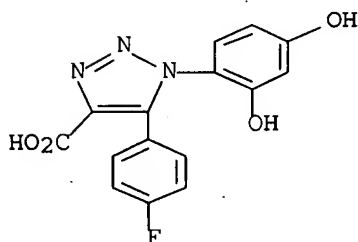
prepd. as heat shock protein 90 (HSP90) inhibitors. Thus, 5-chloro-2,4-dimethoxyphenylamine was treated with NaNO_2 in the presence of H_2SO_4 followed by the addn. of NaN_3 . The resultant azide underwent cyclization with 3-(4-fluorophenyl)-3-oxopropionic acid Me ester gave intermediate II ($\text{X} = \text{OMe}$, $\text{R} = \text{OH}$). Demethylation of this compd. with 48% HBr followed by esterification with EtOH yielded triazolecarboxylate II ($\text{X} = \text{OH}$, $\text{R} = \text{OEt}$), which showed $\text{IC}_{50} < 10 \mu\text{M}$ for binding to HSP90 in a fluorescence polarization assay. Therefore, I and their compns. are useful for immunosuppression or the treatment of cancers, viral disease, inflammatory diseases and so on.

IT 820232-70-0P, 1-(2,4-Dihydroxyphenyl)-5-(4-fluorophenyl)-1H-[1,2,3]triazole-4-carboxylic acid

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(inhibitor; prepn. of triazolecarboxylates as heat shock protein 90 (HSP90) inhibitors)

RN 820232-70-0 CAPLUS

CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-(2,4-dihydroxyphenyl)-5-(4-fluorophenyl)- (CA INDEX NAME)

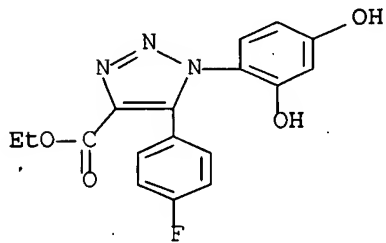


IT 820232-73-3P, 1-(2,4-Dihydroxyphenyl)-5-(4-fluorophenyl)-1H-[1,2,3]triazole-4-carboxylic acid ethyl ester 820232-74-4P, 1-(5-Chloro-2,4-dihydroxyphenyl)-5-(4-fluorophenyl)-1H-[1,2,3]triazole-4-carboxylic acid ethyl ester

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(inhibitor; prepn. of triazolecarboxylates as heat shock protein 90 (HSP90) inhibitors)

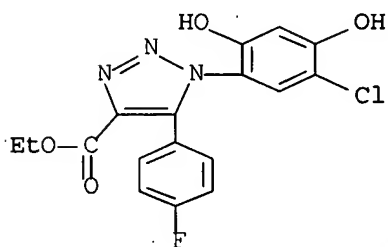
RN 820232-73-3 CAPLUS

CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-(2,4-dihydroxyphenyl)-5-(4-fluorophenyl)-, ethyl ester (CA INDEX NAME)



RN 820232-74-4 CAPLUS

CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-(5-chloro-2,4-dihydroxyphenyl)-5-(4-fluorophenyl)-, ethyl ester (CA INDEX NAME)



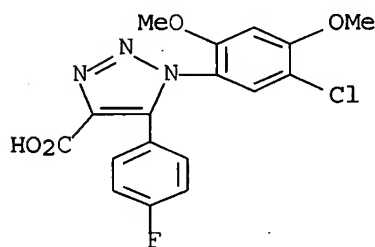
IT 820232-72-2P, 1-(5-Chloro-2,4-dimethoxyphenyl)-5-(4-fluorophenyl)-1H-[1,2,3]triazole-4-carboxylic acid

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of triazolecarboxylates as heat shock protein 90 (HSP90) inhibitors)

RN 820232-72-2 CAPLUS

CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-(5-chloro-2,4-dimethoxyphenyl)-5-(4-fluorophenyl)- (CA INDEX NAME)



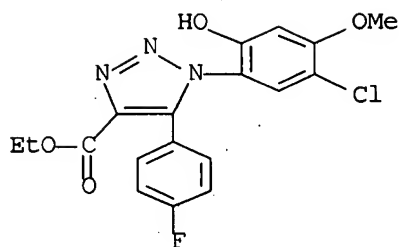
IT 820232-75-5P, 1-(5-Chloro-2-hydroxy-4-methoxyphenyl)-5-(4-fluorophenyl)-1H-[1,2,3]triazole-4-carboxylic acid ethyl ester

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of triazolecarboxylates as heat shock protein 90 (HSP90) inhibitors)

RN 820232-75-5 CAPLUS

CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-(5-chloro-2-hydroxy-4-methoxyphenyl)-5-(4-fluorophenyl)-, ethyl ester (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:363009 CAPLUS Full-text

DOCUMENT NUMBER: 140:399359

TITLE: 1,5-Diarylsubstituted 1,2,3-triazoles as potassium channel activators. VI

AUTHOR(S): Biagi, Giuliana; Calderone, Vincenzo; Giorgi, Irene; Livi, Oreste; Martinotti, Enrica; Martelli, Alma; Nardi, Antonio

CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Pisa, 56126, Italy

SOURCE: Farmaco (2004), 59(5), 397-404

CODEN: FRMCE8; ISSN: 0014-827X

PUBLISHER: Editions Scientifiques et Medicales Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:399359

AB As part of our program toward designing potassium channel openers, synthesis of a novel series of 1,5-di-Ph substituted 1,2,3-triazoles, as potential activators of the large-conductance calcium-activated potassium channels (BK), as well as their vasorelaxant activity are presented. The functional effect of these potential structurally novel BK-openers on vascular contractile function were studied in vitro, using isolated rat aortic rings pre-contracted with KCl 20 mM. Among the target compds., only 16 showed appreciable effectiveness, exhibiting an efficacy parameter (57%) lower than that of NS1619 and a comparable potency index (pIC50: 5.58).

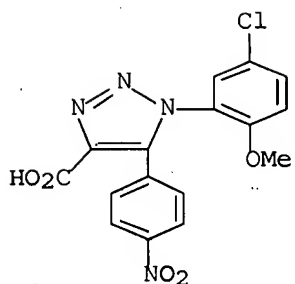
IT 690638-34-7P 690638-38-1P 690638-39-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and vasorelaxant activity of 1,5-diarylsubstituted 1,2,3-triazoles as potassium channel activators)

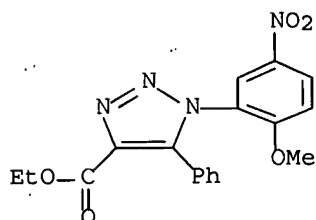
RN 690638-34-7 CAPLUS

CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-(5-chloro-2-methoxyphenyl)-5-(4-nitrophenyl)- (CA INDEX NAME)



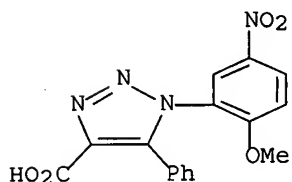
RN 690638-38-1 CAPLUS

CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-(2-methoxy-5-nitrophenyl)-5-phenyl-, ethyl ester (CA INDEX NAME)



RN 690638-39-2 CAPLUS

CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-(2-methoxy-5-nitrophenyl)-5-phenyl-, ethyl ester (CA INDEX NAME)

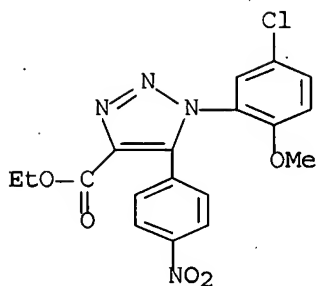


IT 690638-37-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis and vasorelaxant activity of 1,5-diarylsubstituted
1,2,3-triazoles as potassium channel activators)

RN 690638-37-0 CAPLUS

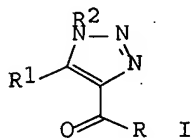
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-(5-chloro-2-methoxyphenyl)-5-(4-nitrophenyl)-, ethyl ester (CA INDEX NAME)



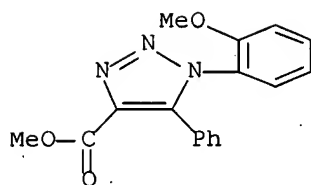
check prior art.
No utility, not 103a.

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1994:270233 CAPLUS Full-text → check 102b
 DOCUMENT NUMBER: 120:270233
 TITLE: 1,3-Dipolar cycloaddition of o-substituted phenyl azides to 1-aryl-3-phenylprop-2-yn-1-ones and methyl 3-arylprop-2-ynoates
 AUTHOR(S): Kandeel, K. A.; Youssef, A. S. A.; Fouli, F. A.
 CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt
 SOURCE: Afinidad (1993), 50(447), 316-18
 CODEN: AFINAE; ISSN: 0001-9704
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

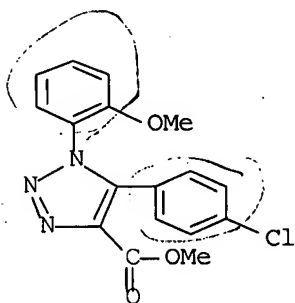


AB Dipolar cycloaddn. of 2-methoxyphenyl azide and 2-chlorophenyl azide with 1-(aryl)-3-phenyl-2-propyn-1-ones gave 1-(aryl)-4-(aryloxy)-5-phenyl-1,2,3-triazoles I (R-R2 = Ph, substituted phenyl) as the major products. On the other hand, 2-nitrophenyl azide failed to react with 1-(aryl)-3-phenyl-2-propyn-1-ones.
 IT 154581-28-9P 154581-29-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, from Ph azide and (aryl)propynone)
 RN 154581-28-9 CAPLUS
 CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-(2-methoxyphenyl)-5-phenyl-, methyl ester (9CI) (CA INDEX NAME)



RN 154581-29-0 CAPLUS

CN 1H-1,2,3-Triazole-4-carboxylic acid, 5-(4-chlorophenyl)-1-(2-methoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)



=>

=>

Executing the logoff script...

=> LOG H

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

22.02

1266.19

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-3.12

-52.26

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 13:07:29 ON 12 OCT 2007